



A tool for diffusion simulations

1 Introduction

DICTRA is a general software package for simulation of Diffusion Controlled TRAnsfOrmations in multicomponent alloys. The DICTRA software is based on a numerical solution of the multicomponent diffusion equations. DICTRA is interfaced with Thermo-Calc, which handles all necessary thermodynamic calculations. The diffusion simulations are based on assessed kinetic and thermodynamic data, which have been stored in databases. Up to 10 components may be treated simultaneously in a simulation, provided that the necessary kinetic and thermodynamic data is available.

In the development of DICTRA, emphasis has been placed on linking fundamental methods to critically assessed thermodynamic and kinetic data, allowing simulations to be performed with realistic conditions on alloys of practical importance. The simulations are one-dimensional and three different geometries, cylindrical, spherical and planar can be used. This is sufficient to model many cases of interest. The cylindrical geometry can e.g. be used both for modelling of diffusion in a tube wall as well as the dissolution of a rod-shaped precipitate.

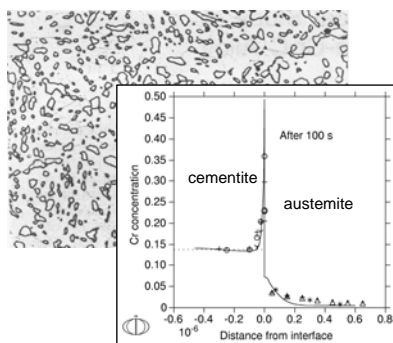
DICTRA is the result of more than 20 years and 60 man-years research and development at KTH in Stockholm, Sweden and joint efforts with the Max-Planck Institute für Eisenforschung in Düsseldorf, Germany. International collaborations with many R&D partners and constructive suggestions from users have also contributed to its development.

The first commercial version of DICTRA was released in 1995. Since then there have been regular updates and improvements.

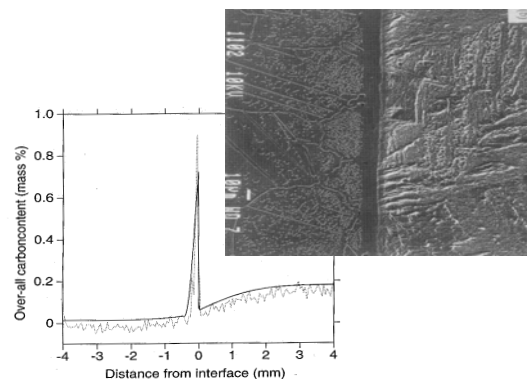
Today DICTRA is a well recognised research tool for materials and process development, used daily by engineers and scientists all over the world.

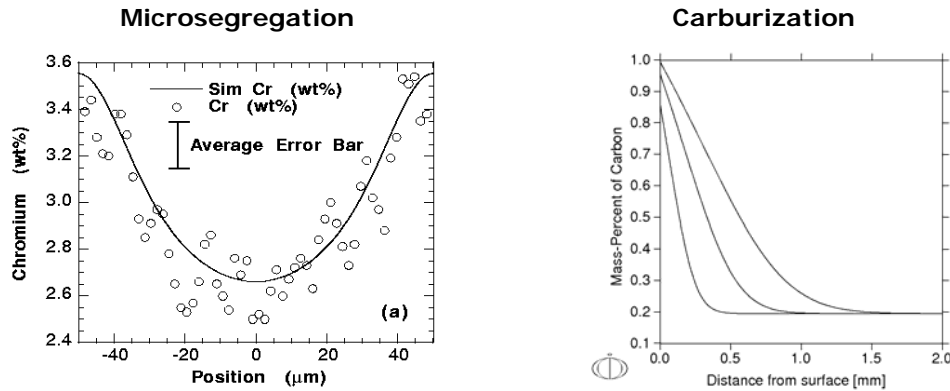
Some DICTRA application

Carbide dissolution



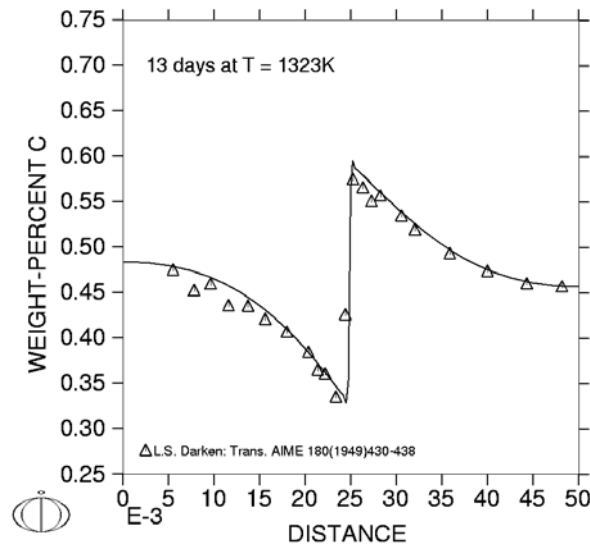
Carbon diffusion between two Steels





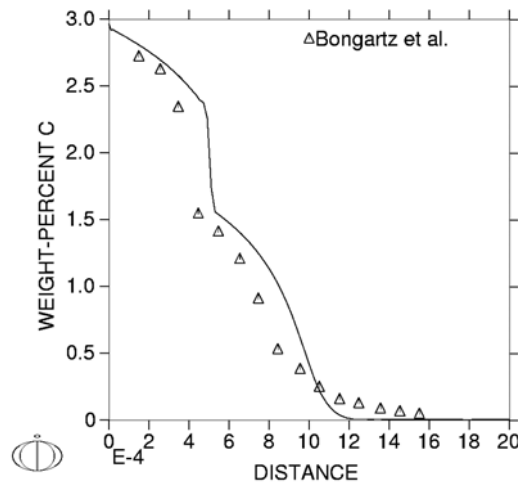
2 The DICTRA software

The accurate description of multicomponent diffusion in DICTRA makes it possible to account for processes such as up-hill diffusion. A simulation of the historical Darken experiment with a joint of two steels with initially similar carbon contents but different silicon contents is shown below. The higher silicon content in the left part of the figure increases the carbon activity, which causes carbon to diffuse to the right. A discontinuity in carbon content is seen at the gradient in silicon content.



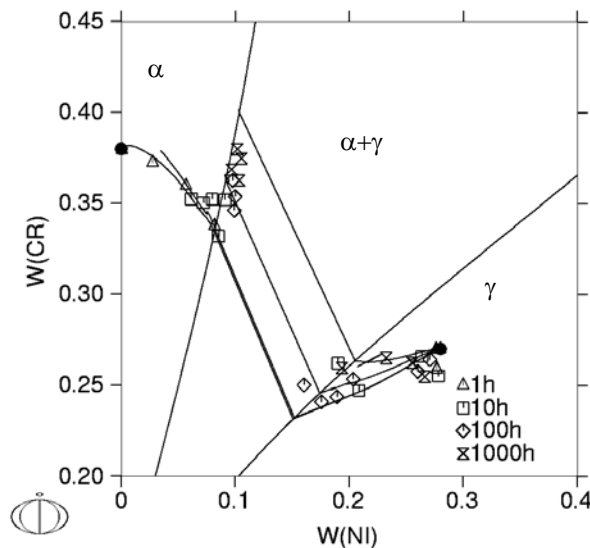
Concentration profile for carbon in a joint between two steels with different Si contents. The symbols are experimental data from L.S. Darken (1949).

DICTRA's coupling to Thermo-Calc provides access to accurate multicomponent thermodynamics and phase equilibria making it possible to simulate e.g. diffusion in dispersed systems where precipitates act as sources and sinks of diffusing elements. Below is an example where an Ni-25Cr alloy is carburized. The carbon diffusion causes precipitation of M_3C_2 , M_7C_3 carbides and the concentration profile below is far from the common error-function solution that could have been expected.



Concentration profile for carbon in a carburised Ni-25Cr alloy. The symbols are experimental data from Bongartz *et al.* (1986).

The flexible post-processor in the software makes it possible to use many different axis quantities such as concentration, distance, time, activity, chemical potential and user defined functions in the plots. Illustrative diffusion paths as below are easily plotted.



Diffusion path for a ternary Fe-Cr-Ni diffusion couple. Symbols are experimental data from Kajihara *et al.* (1993)

2.1 Applications

The DICTRA software has been applied to several problems of scientific and practical interest such as:

- Solidification and microsegregation in steels
- Gradient sintering of cemented carbides
- Coarsening of γ' -precipitates in nickel base alloys
- Carburization and decarburization of steels
- Carburization of High-Temperature alloys
- Nitriding and Nitrocarburizing of steels
- Austenite/ferrite diffusional transformations in steels
- Generate input for construction of TTT- and CCT-diagrams
- Interdiffusion in coating/substrate compounds
- Growth of pearlite in alloyed steels

And much more, see our reference list for detailed information.



2.2 User Interface

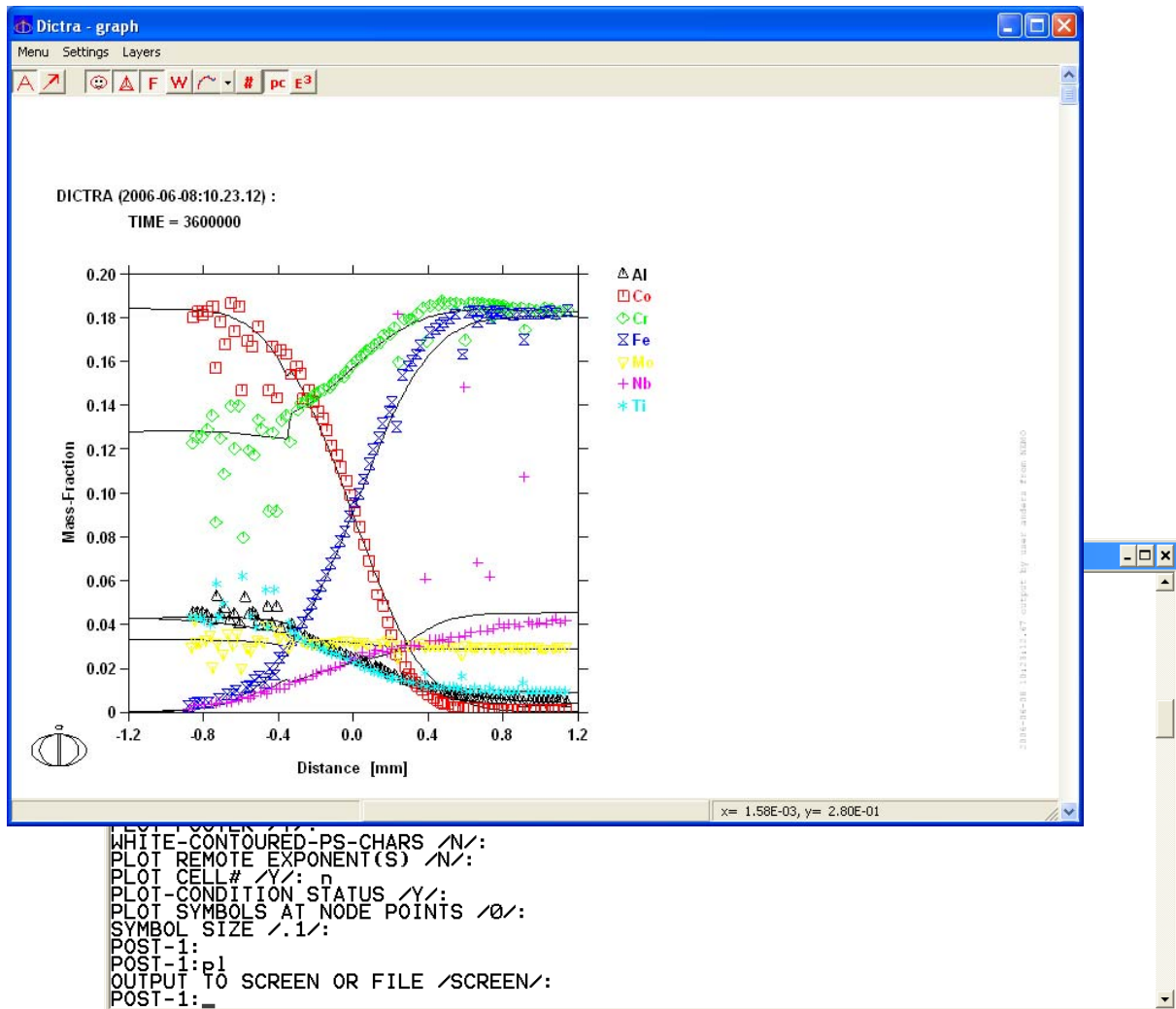
The DICTRA software is divided into several different modules for performing different tasks, e.g. retrieving data, setting up a simulation, or plotting the results. The user interface is very similar to the user interface in Thermo-Calc Classic, with a command line interface where commands are typed. All commands can be abbreviated for convenience.

After gaining some experience with the software, it is possible to construct macro-files, which sets up and executes a simulation. Virtually all experienced users use macro-files since it's possible to set up a simulation in a very short time (minutes) using this feature.

There are complete help facilities for the users. A list of available commands can be retrieved by simply typing a question mark ? at the command prompt. A description of all commands is also available on-line.

2.3 Output Facilities

DICTRA has a post processor for producing outputs from the simulations. Graphs are easily plotted with different axis variables. The post processor supports different graphical formats such as EMF, PNG, BMP, PDF, JPEG, TIFF, PostScript, HPGL, HP-Laserjet, Regis etc. and many others. The co-ordinates of the plot can also be printed on a file to be processed by other software.



2.4 Availability of DICTRA

The DICTRA software is available for most modern computer systems. A list of the computers and O/S that the software is available for is given below.



2.5 Computers and O/S that the DICTRA software is available for

Computers		O/S	Version
PC		Windows	NT4/2000/XP
			95/98/Me
		Linux	
UNIX-Platforms	SUN	SOLARIS	
	SGI	IRIX	

2.6 From Atomic Mobility to Various Diffusivities

In a DICTRA simulation, the multicomponent diffusion equations:

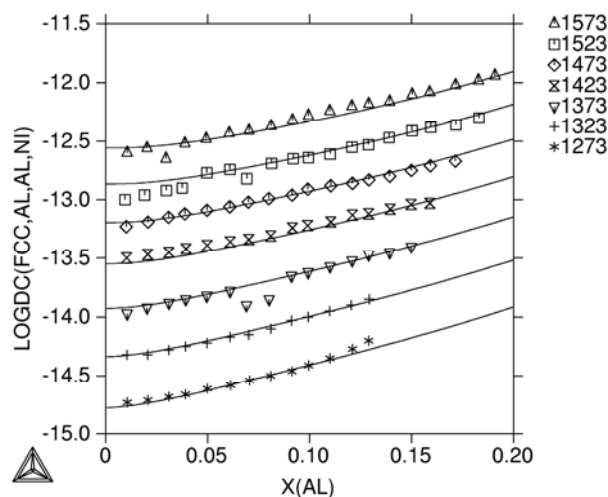
$$J_k = - \sum_{j=1}^{n-1} \tilde{D}_{kj}^n \frac{\partial c_j}{\partial z}$$

are solved, using a complete, (n-1)x(n-1) temperature and concentration dependent diffusivity matrix \tilde{D}_{kj}^n . The diffusivity matrix is calculated from parameters stored in a mobility database and a thermodynamic database. The thermodynamic databases are the same as used by Thermo-Calc.

The mobility databases are created through an assessment procedure similar to the one for thermodynamic databases. Experimental data are collected and selected from the literature. Parameters in the mobility models are optimised to give the best possible description of the experimental data. The optimised parameters are then stored in a mobility database.

DICTRA contains a module for optimisation of mobility data, PARROT. This module enables the user to expand existing databases as well as creating own databases. Demonstration examples and documentation for this is available in the DICTRA User's Guide and Calculation Examples.

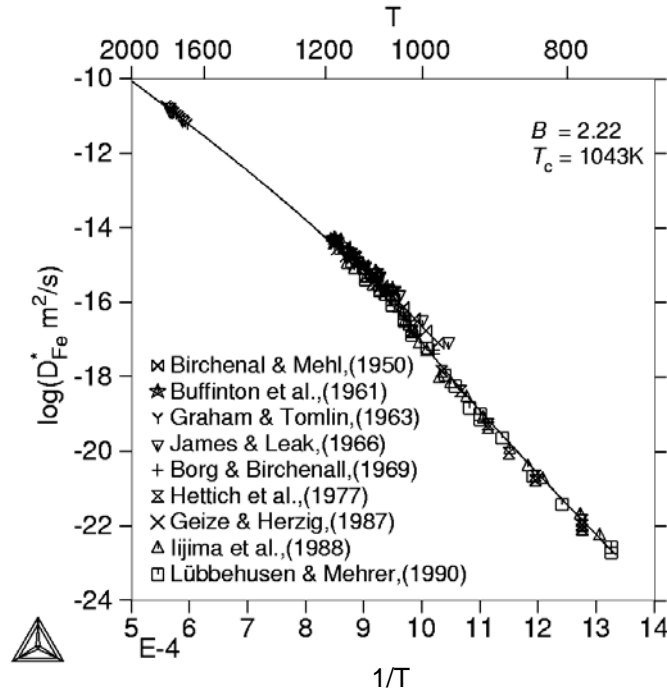
Using the mobility databases it is possible to calculate e.g. tracer-, self-, intrinsic- and interdiffusivities. The diffusivities are normally temperature and concentration dependent as shown below.



Logarithm of the interdiffusion coefficient (\tilde{D}) in the FCC-phase of the Ni-Al system as a function of x_{Al} for different temperatures (1273, 1323, 1373, 1423, 1473, 1523 and 1573 K). Solid lines are calculated using DICTRA and the symbols are experimental measurements.



In DICTRA, an effort has also been made to incorporate other effects on the diffusivities. The ferromagnetic transformation occurring in e.g. BCC-Fe has a marked effect on the diffusion in this phase. This is practically important in e.g. steels and a model for the effect of the ferromagnetic transformation on the diffusivities is implemented in DICTRA as shown below.



Logarithm of the self diffusion coefficient of iron plotted against the inverse of temperature. Note the deviation from linearity around the Curie temperature 1043 K. The solid line is calculated using DICTRA and the symbols denote experimental measurements.

2.7 Mobility Databases

Mobility databases for different types of alloys are available from Thermo-Calc Software. For a list of currently available mobility databases, please visit our homepage <http://www.thermocalc.com>

3 More Information

You can download the DICTRA Users Guide and Examples Book for free from our website and have a closer look at the program. If you have more questions or would request any support or guidance in the selection of databases, please do not hesitate to contact us.

